California Institute of Technology – Center for Simulating Dynamic Response of Materials

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Integrated simulation capability

Subproject description

The primary goal of the Center is developing an integrated simulation capability referred to as the Virtual Test Facility (VTF), a suite of computational engines capable of conducting high-performance computations relevant to the simulation of high velocity impact experiments. The chief components are: a 3-D parallel unigrid Eulerian solver with level set capability, a 3-D parallel Adaptive Mesh Refinement (AMR) Computational Fluid Dynamics (CFD) solver utilizing the Grid Adaptive Computational Engine (GrACE) adaptive grid environment, a 3-D parallel Lagrangian solid mechanics solver with adaptive meshing, facilities for checkpointing and visualization, and a Python scripting environment (Pyre) to integrate the computational engines and provide a uniform environment for running the simulations. In addition, the VTF implements a fluid-solid coupling algorithm that employs level set technology to enable coupled simulations in which the fluid mechanics is performed using the Eulerian facility, and the solid mechanics is performed using the Lagrangian facility.

FY03 accomplishments

We have initiated integrated simulations using the VTF for shock focusing leading to converging shocks. These studies address issues of both shock stability as well as generation of compressible turbulence due to Richtmyer-Meshkov (R-M) instabilities. A related experimental effort will provide valuable design insight as well as simulation validation. A second integrated simulation incorporates the multiscale model for Tantalum based on a phase-field approach to dislocation dynamics to achieve a direct numerical simulation of polycrystals. The existing fluid solver is undergoing a redesign as a collection of cooperating components that are assembled by the integration framework under the user's direction. In support of our research in gas phase detonation and mixing we are augmenting our existing solver to model reacting flows with explicit chemistry in a scalable way. We are continuing the development of our parallel fracture and fragmentation capability including parallel contact. We are also currently exploring the extension of the fluid-solid coupling algorithm to the case where fragmentation occurs in the solid. Finally the provision of release and configuration management in Python is in progress and should be complete by Q4 FY03.

Plans for FY04 and beyond

In FY04, we will provide complete support for scalable contact, fracture and fragmentation. We will complete development of the component based fluid solver that will implement a new thermodynamic state cache to speed up multi-species chemistry computations. Visualization support, flexible simulation control and full simulation archiving will be implemented in Pyre. These capabilities will be used to accomplish a fully coupled simulation of detonation-induced fracture in metal tubes. In FY05 we will complete a component based redesign of the solid solver to make it totally compliant and steerable by Pyre. The level set algorithm will be redesigned so as to be totally scalable for large solid meshes. We will perform integrated simulations of plate impact with advanced modeling. We will demonstrate a grid-aware version of Pyre and will provide the first release of the Pyre software. In FY06 an adaptive tetrahedral meshing capability based on variational techniques will be completed and integrated into the solid solver. An adaptive variational integrator capability will also be integrated into the solid solver. In addition, we will integrate automated reliability mechanisms to enable scalable (and reliable) simulations on thousands of processors. In the area of integrated simulation we will accomplish a converging shock simulation with turbulence modeling. In FY07, the VTF will be a full-featured grid aware framework. Integrated, validated simulations to be completed during this period include: plate impact, converging shocks, and detonation-induced fracture.

Compressible Turbulence and Combustion

Subproject description

In this subproject, 3-D, unsteady simulations of nonpremixed turbulent combustion will be executed with increasing complexity in geometry, in the level of modeling of turbulence dynamics and turbulent mixing across the range of scales, and in the level of detail in the chemistry modeling. The relevant codes will be operated in parallel mode on ASCI platforms. In the area of compressible turbulence, new numerical methods and algorithms are being developed that are suitable for use in the large-eddy simulation of compressible and shock-driven turbulence. The target problem is the strong-shock R-M instability with re-shock from the end wall implemented in an AMR setting within the VTF. We are currently also using DNS to study mixing in Rayleigh-Taylor (RT) instability. This will increase our understanding of buoyancy-driven, variable-density, inhomogeneous, anisotropic turbulence and turbulent mixing. Analysis of full DNS data sets will be used to develop and test subgrid-scale (SGS) models for anisotropic turbulent mixing. We are also using numerical simulation as a tool to improve our understanding of the structure and dynamics of detonation waves in gases. The goal is to simulate these flows using massively parallel platforms. This will require direct numerical simulation that ultimately resolves the motion down to the level of viscous dissipation, realistic representation of the chemical kinetics, and 3-D motion.

FY03 accomplishments

A very large 3-D DNS of the non-premixed reacting turbulent jet has been partially completed. This simulation contains of order 10^8 grid points at a Taylor Reynolds number of order 50, and at finite Damköhler number. The chemistry is Peter's four-step reduced mechanism for Methane. This will be used to develop new sub-grid models for turbulent combustion. A hybrid numerical method has been developed based on use of a Weighted-Essentially Non-Oscillatory (WENO) method near shocks and an optimized centered-difference stencil (OCD) in smooth turbulent regions away from shocks. The hybrid method works well for decaying compressible turbulence and is now being tested in 3-D RM instability simulations. A detailed study of composition statistics computed from DNS data of incompressible RT instability between miscible fluids has been made. The simulations achieve outer-scale Reynolds numbers in excess of 3000, but well below the mixing transition. Computations are being carried out on projectile-initiated detonation using the GEL method and a novel starting technique based on time dependent heat release. The

simulations have used both detailed and one-step chemical kinetic models. The critical conditions for detonation stabilization are being analyzed using the critical decay rate model and transformation of coordinates to obtain spatial derivatives along streamlines.

Plans for FY04 and beyond

In FY04 we will complete an LES calculation of the plane turbulent jet at large Reynolds numbers. We will also complete a DNS of the weak shock R-M instability. Finally, a 2-D simulation of viscous detonation using a simplified reaction model will be completed. In FY05 we will complete an LES/DNS of the 3-D axisymmetric turbulent jet using turbulence models developed at the center. We will also complete a simulation in 3-D of viscous detonation again using a simplified reaction model but which will exhibit weak instability. In FY06 we will incorporate an ILDM modeling approach into the turbulent combustion capability of the VTF. We will complete a full 3-D simulation of weak-shock R-M instability. We will also achieve a 3-D simulation of viscous detonation using a reduced chemistry capability that is weakly stable. In FY07 a full LES of cylindrical and spherical strong shock R-M instability will be accomplished along with a 3-D viscous detonation propagation with reduced chemistry.

Solid Dynamics

Subproject description

The Solid Dynamics effort is structured in accordance with the multiscale modeling paradigm, with activities ranging in scale from the quantum-mechanical realm to full-scale engineering systems and components. The scope and main target areas of the project for FY04 are shock-induced dynamic fracture, spallation and fragmentation in metals, including model systems such as Al and Li, and materials such as U_6Nb, the dynamics of shocked BCC metals, with particular focus on materials such as Fe and U_6Nb exhibiting coupled martensitic transformations and plasticity. Additional overarching goals of the solid dynamics project are the development of scalable solution procedures enabling high-fidelity integrated simulations of multi-component engineering systems within the VTF (in collaboration with the CS and Integration groups), and the validation and verification of all models of material behavior and numerical algorithms developed under the project.

FY03 accomplishments

- Development and verification of a generalized saddle-point search engine. The saddle-point engine will minimize the stress along transition paths and will permit the optimization of the cell shape, as required for the study of martensitic phase transformations.
- Development and verification of serial tight-binding model for transition metals. We will develop a fast and accurate tight-binding method suitable for transition and other metals, including non-collinear magnetism. The model will be calibrated for Fe.
- Development of a level-set code for the simulation of nanovoid coarsening. We will develop a level-set code for simulating the diffusive coarsening of a vacancy/nanovoid distribution, accounting for temperature and pressure. We shall verify the correctness of the code for analytically tractable spherically symmetric configurations and calculate critical-void nucleation rates.
- Development of DNS polycrystalline capability. We shall complete the VTF implementation of polycrystal simulation capability based on the explicit resolution of the grains, including large-scale calculations for polycrystalline Ta demonstrating the feasibility of the approach and its ability to account for microstructural effects such as inhomogeneity of plastic deformation within the grains, and grain size and morphology.

- Integration of continuum spall model into the VTF. We will integrate the continuum spall model and spall element into the VTF and conduct validation studies. We shall verify the correctness of the code by means of ring-expansion and plate-impact tests.

Plans for FY04 and beyond

The saddle-point engine developed in FY03 will be applied to the calculation of polymorphic phase-transition paths in Fe. In addition, the energy of Fe twin boundaries will be calculated ab initio. In FY04 we will develop a tight-binding model for transition metals via replacement of the inner self-consistency loop for the determination of the magnetic moments by a Car-Parrinello-like method. This replacement is expected to speed-up calculations by a factor of about 10. We will continue to develop a level-set code for simulating void growth and coalescence by including lattice defects such as dislocations and grain boundaries. We will also validate the DNS polycrystal capability using the multiscale model of Ta and accounting for subgrain dislocation structures. We shall complete the analysis of nanovoid cavitation in BCC metals using the quasi-continuum method coupled to dislocation dynamics and we will complete the integration of the polymorphic Fe model into the VTF, including consideration of mixed states and the influence of shear on the transition points.

Materials Properties Methodology

Subproject description

A key feature of our effort is to determine all input data to be used in the VTF from first principles theory and computation. Thus the Materials Properties (MP) team, led by William A. Goddard, III, develops and enhances methods for the accurate prediction of materials properties from first principles and will integrate both the methods and the results into the VTF. In order to achieve these goals, the MP team will: continue developing the technology required to predict these properties from first principles, validate the accuracy of the properties by comparison to relevant experiments, and develop empirical corrections to the first principles results as needed to improve matches with experiment. We will also implement this computational technology on massively parallel computers across different platforms and incorporate the MP software, scripts, and data into the Materials Properties Facility (MPF), a component of the VTF.

FY03 accomplishments

We are currently developing a simple Quantum Monte-Carlo (QMC) facility for heats of formation of simple systems; QMC techniques sample the many-particle equations rather than approximating them with a set of coupled one-particle equations. QMC techniques are in theory exact, but enormous amounts of computational time are required to converge the sampling of the QMC simulation. By the end of FY03, we will have overcome several of these impediments. In particular, we will complete development of a parallel QMC code (perfectly scaling up to 2048 processors) and a statistical analysis techniques for analyzing QMC results, as well as implement a state-of-the-art techniques for variational and diffusion QMC allowing fast convergence of many-electron correlation functions. In FY03 we have been working toward the development of a Python integration layer (the MPF) that will unify different elements of the atomistic simulation software used in the MP group. The MPF will enable these tools to be submitted from a common interface, such as the VTF, which will allow the materials properties to be integrated into the VTF. In addition, it will allow the tools themselves to be integrated into the VTF, which will allow VTF users to develop additional materials properties as needed. Our ASC effort has made a breakthrough: the development of a reactive FF (ReaxFF) that allows an accurate description of complex chemistry (including all of the intermediates and barrier heights). In FY03 we are developing a systematic form of ReaxFF that can be used for a range of energetic material (RDX, HMX, TATB, and PETN) and we are extending it to metal alloys and oxides.

Plans for FY04 and beyond

In FY04 our plan is to systematize the ReaxFF procedure so that non-experts can construct reactive force fields. We also plan to fully integrate the MPF facility into the VTF. In addition we will build in the parameters for new materials required by the VTF. In FY04 we will apply QMC to chemical systems such as RDX that are relevant to ASC applications in HE and SD. This will be used to gauge the level of accuracy these techniques can provide in a practical computing environment, which will be used to drive the development of improved methods through which we can accelerate the process. Among these improvements, we will investigate techniques to simulate only a pair of electrons at a time, to use post-Hartree-Fock (HF) correlation techniques to approximate the static correlation in the chemical systems better than done with the traditional single determinant. In FY05 we will improve and extend the functionality and capability of the proposed MPF. We will also begin consideration of the single node performance of the ReaxFF. We will also examine the scalability of the parallel computation with the goal of increasing efficiency. In FY06 we will extend the development of the ReaxFF model to systems of interest to the Solid Dynamics group and include imperfections such as inclusions, defects etc. To further our effort in the area of QMC, we will extend this to include frozen HF/DFT core wave functions. In FY07 we will provide a fully validated MPF within the VTF framework. We will also complete ReaxFF simulations of heterogeneous composites of metals, oxides, explosives, and polymers. Finally we will implement multiconfiguration QMC for excited states.

Validation

Subproject description

Validation plays an integral role in the proposed scientific program. As part of our ASC program we have designed a set of experiments in the areas of compressible turbulence, detonation, and solid dynamics that examine key phenomena of interest to the ASCI program. In addition, each of our end-to-end integrated simulations is tied to an experiment aimed at validating the entire simulation. At the end of FY07, we plan to have a validated simulation capability for each of the experiments that are currently being designed.

Richtmyer-Meshkov instability in converging geometry - These experiments validate our integrated simulation of R-M instability in converging geometries. They will demonstrate a method for generating 2- and 3-D converging shocks and shock focusing. We will also facilitate understanding of the stability of converging shocks through these experiments.

Detonation-driven fracture - These experiments will test the ability of the VTF to simulate stress waves in thin shells and dynamic fracture. The experiments are designed to explore crack bifurcation, detonation waves in gases, and shock waves in the surrounding air.

Impact dynamics of single and polycrystals - These impact experiments are directed at microstructural characterization of single- and poly-crystal deformation at various strains, strain rates and temperatures. The resulting data provide validation for the atomistic and quasi-continuum models that are essential to our program for multiscale modeling of solids.

FY03 accomplishments

Richtmyer-Meshkov instability in converging geometry – Preliminary simulations have examined shock propagation in a converging geometry using various interfacial shapes to diffract the shock. These simulations will guide design validation experiments for the project. We anticipate demonstrating shock wave propagation in a converging geometry by 4Q FY03.

Detonation-driven fracture -In FY03 we have obtained strain, pressure, and crack speed records of pre-flawed aluminum tubes under gaseous detonation loading as well as visual documentation of post-test specimens and crack paths. In work to be completed this year, we will

consider hydrostatic, deflagration, and DDT loading of pre-flawed metal tubes with the same diagnostics. Planning for integrated simulation is underway.

Shock-induced dynamics of single- and poly-crystals -We have initiated dynamic mixed-mode fracture-failure experiments of C-300/HSLA steels. These are drop-weight experiments using high-speed photography for diagnostics. Dynamic fragmentation experiments in C-300 and sandwich structure geometries are also in progress.

Plans for FY04 and beyond

Richtmyer-Meshkov instability in converging geometry – In FY04, we will perform experiments on shock propagation and shock stability in coordination with simulations. These experiments will look at shock diffraction as well as shock stability in a converging geometry. In FY05, we will examine the R-M instability by running shock waves though perturbed interfaces. These experiments will provide important validation information for a set of matching simulations. In future years we will examine possible strong shock interactions in which the solid casing of the shock tube will be important in shock evolution.

Detonation-driven fracture – In FY04, we will implement Schlieren one-axis imaging of the shock emerging from aluminum tubes ruptured by gaseous detonations. We will also image caustics of the propagating cracks in polycarbonate tubes ruptured by gaseous detonations. Two-axis imaging will be employed in FY05.

Impact dynamics of single- and poly-crystals – In FY04, we will complete experiments on low velocity perforation of steel plates using high-speed photography. We will also measure the fraction of conversion of plastic work to heat in iron as a function of strain and strain rate at high temperatures. In FY05, we will perform high velocity perforation experiments in iron as well as imaging of shear banding at high velocities using combined photography/thermography. Experiments on the effect of loading history in iron at high temperatures and large strains will also be performed. All validation data will be available for use in future simulations.

Stanford University – Center for Integrated Turbulence Simulation

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Overview The Stanford ASCI Center is developing high-fidelity simulation capability for flow in aircraft gas turbine engine and a new supercomputer concept for scientific applications, termed the streaming supercomputer.
The project is organized into four groups: the combustor group, the turbomachinery group, the integration group and the streaming supercomputer group.
Progress during FY03 and plans for FY04 are given below for each group.

Combustor Group

The combustor group is developing an LES unstructured code, CDP, for simulating reacting multiphase flows in realistic aircraft engine configurations. The CDP code was successfully applied to the simulation of the non-reacting flow in a $1/18^{th}$ sector of a Pratt & Whitney (PW) combustor. Reacting multiphase flow simulations were initiated in coaxial combustor geometries. Scalability studies were conducted on DOE computers up to 1,000 processors.

FY03 Accomplishments for the Combustor Group

Code and algorithm development: A major effort in rewriting the kernel of CDP is well under way. This effort was considered critically important to achieving high performance for very large simulations: the estimated computational grid required to perform a complete PW engine combustor simulation is 100 million unstructured control volumes. The main feature of the new code, CDP-α, is a flexible data management strategy. This will allow the implementation of dynamic load balancing, mesh adaptation, and rapid implementation of new physical modules. The initial tests of CDP-α show substantial performance improvements (memory and speed) over CDP. Time-to-solution is still recognized as a pacing item and further algorithm developments are on-going (multigrid). A parallel preprocessor was developed to manage very large meshes.
Validation: Cold flow simulations for the PW combustor geometry and for the PW unconfined rig geometry were completed. Agreement with the available experimental data was satisfactory. A secondary breakup model was tested in a PW injector geometry and compared with available measurements showing good agreement. Additional comparisons with RANS predictions showed substantial improvements. An evaporation model was also validated in a coaxial combustor geometry; excellent agreement with available data was obtained. A chemical table

(flamelet library) corresponding to JET-A fuel was generated, and a reacting flow simulation in the PW combustor at operating conditions is under way.

Combustion Science: Combustion in aircraft engines is essentially non-premixed, but premixed and partially-premixed combustion play central roles in the flame stabilization region. An entirely new LES formulation of the level-set method for premixed turbulent combustion has been developed. Excellent agreement with experimental data is observed in the application of the model in LES of turbulent premixed Bunsen flames.

The Flamelet/Progress Variable approach was successfully validated with experimental data, and has recently been implemented in the CDP code. Reacting flow simulations in a coaxial combustor geometry using this approach are well under way, and are being compared to both experimental data and structured-grid LES computations. To extend the model for application to flows where local flame extinction and re-ignition are important, the model has been applied in an a priori study using data from the DNS of non-premixed combustion in isotropic decaying turbulence, where extinction and re-ignition are important. Shortcomings of the model have been identified in this study, but we are working to eliminate them.

Spray Modeling: A stochastic model for secondary breakup along with hybrid particle/parcel approach for Lagrangian Particle Tracking (LPT) was developed and validated in a realistic PW injector geometry against the experimental data. The total number of tracked computational particles was effectively reduced by the hybrid model (3 million particles represented 15 million droplets). A droplet evaporation model has been implemented and validated. LES along with LPT provided accurate predictions of droplet dispersion and rates of evaporation. The droplet evaporation and breakup models are now coupled with the flamelet/progress variable approach to perform spray flame simulations in realistic PW combustor geometries.

FY04 Goals for the Combustor Group

Multigrid: Complete the CDP-α kernel, including full multilevel multigrid implementation with a diffusion based agglomeration strategy for the Poisson and other transport equations.

Mesh Refinement: Develop and implement local mesh refinement based on quasi-homothetic element decomposition. Develop a turbulence-statistics-based adaptive criterion for LES.

Dynamic Load Balancing: Implement dynamic load balancing to address the computational imbalance introduced by spray breakup simulations in complex geometry using LPT.

Variable Density Formulation: Investigate the accuracy and stability of different low-Mach number variable-density formulations for unstructured grid reacting flow simulations.

Validation: Validate the combustion-spray-evaporation modules of CDP for the reacting flow in both coaxial combustors and $1/18^{th}$ sector of the PW combustor.

Combustion Science: Extend Flamelet/Progress Variable approach to describe extinction/re-ignition. Incorporate accurate modeling of NO_x, including a radiation model. Validation with experiments in aircraft engine model combustor experiment.

Eulerian/Lagrangian Multiphase Model: Develop a hybrid level set Eulerian-Lagrangian approach to capture the liquid fuel interface and more accurately model primary atomization.

Turbomachinery Group

The efforts of the turbomachinery group are focused on the development of highly efficient algorithms and advanced physical models for the solution of the Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations in compressors, turbines and the secondary flow system. A number of phenomena that occur in turbomachinery are dominated by unsteadiness in complex

geometries. More efficient algorithms can have an enormous influence on computational analysis of these problems. Our main objective is to make this possible in a design environment through combinations of new algorithms, better parallel implementations, and sustained collaboration with the Streaming Supercomputer Group. Physical models are being improved to better resolve important phenomena such as roughness, rotation, transition and buoyancy effects on turbulent transport.

FY03 Accomplishments for the Turbomachinery Group

During FY03 we have completed three-dimensional inviscid studies of two promising algorithms: LU-SGS (LU Symmetric Gauss-Seidel) and the non-linear frequency domain procedure. Our software system, TFLO, has been completely re-written to better accommodate these and other algorithm improvements, to improve parallel efficiency, and to facilitate both its future implementation in Brooktran and conservative interfacing with URANS and LES solvers.

Algorithmic developments have the potential to contribute an order of magnitude improvement over state-of-the-art URANS solvers. To avoid long time integrations to a periodic steady state, a non-linear frequency domain approach can be used to reduce the cost of an unsteady simulation to that of a handful of steady-state solutions. In addition, the core solver (currently a multigrid, Runge-Kutta scheme) is being replaced by an LU-SGS, which has been shown this year to provide an improvement of a factor of 5 over the most efficient schemes. Implicit, ADI treatment of turbulence models has previously proved faster and more robust than the R-K method.

Our modeling efforts have resulted in a new model for transition simulation. This model meets a need in low-pressure compressor and turbine analysis. High swirl in tip regions and buoyancy effects on rotating turbine blades mandate further physical modeling of turbulent transport. Cartesian methods have been applied to a serpentine passage flow, for which a massive data set exists. This validation effort has proved the ability to use Cartesian methods in internal cooling systems and will be interfaced with TFLO next year.

FY04 Goals for the Turbomachinery Group

Our application work has been refocused to target important problems in engine fluid-thermal applications. Three applications that promise significant impact were selected: NASA's Stage 35 compressor for rotating stall inception; an aero-structural compressor for simulation of forced vibration and high-cycle fatigue; and the E^3 turbine for moving TFLO into the central problems of turbine cooling. In all cases experimental data are available to assess the fidelity of the simulations and physical models. FY04 goals include demonstrating computational speed improvements (5x) from both the non-linear frequency domain and the LU-SGS methods. Work on a third algorithm, the hybrid-ADI scheme, will also commence. Adaptive and local mesh refinement will be added to the Cartesian code. The first three-dimensional simulations of rotating stall will be completed and analyzed. Turbine tip flow computation will be completed and methods to add cooling streams within the TFLO environment will be developed. Better transition, rotational and buoyancy effect capturing will be implemented in the existing turbulence models.

Integration Group

The objective of the integration group is to create the necessary algorithms, software, and frameworks to enable the coupling of distinct flow solvers, such as LES and RANS. This

requirement arises from the fact that the accurate simulation of turbulent reacting flows requires an LES model, while URANS is sufficient for the compressor and the turbine. The coupling must focus on the fundamental need to create information at the compressor exit (URANS-LES) and at the turbine entrance (LES-URANS).

FY03 Accomplishments for the Integration Group
During FY03 we have completed a framework for coupling arbitrary fluid codes in a fully parallel, distributed environment. This framework was developed to couple with the National Combustor Code (RANS-based) but has been extended to support URANS-LES-URANS coupling. Coupling of an LES combustor code and the TFLO solver was demonstrated.

FY04 Goals for the Integration Group
Major FY04 goals include the continued development of the coupling procedures paying particular attention to the theory of conservative interfacing and the theoretical limits that can be attained with solvers that operate on disparate governing equations. We plan to demonstrate coupling between CDP and TFLO with improved local and global conservation.

Streaming Supercomputer Project

The streaming supercomputer project will develop a scientific computer that offers an order of magnitude or more improvement in performance per unit cost compared to cluster-based scientific computers built from the same underlying semiconductor and packaging technology. We expect this efficiency to arise from two innovations: stream architecture and advanced interconnection networks. Organizing the computation into streams and exploiting the resulting locality using a register hierarchy enables a stream architecture to reduce the memory bandwidth required by representative computations by an order of magnitude or more. Hence a processing node with a fixed memory bandwidth (which is expensive) can support an order of magnitude more arithmetic units (which are inexpensive). Because each node has much greater performance (128 GFLOPs) than a conventional microprocessor, a streaming supercomputer can achieve a given level of performance with fewer nodes, simplifying system management and increasing reliability, e.g., A 1-PFLOPs machine can be realized with just 8,192 nodes.

Exploiting recent developments in signaling technology and router architecture, the streaming supercomputer provides a global memory system in which global memory bandwidth is a substantial fraction (1/1 within a board, 1/4 within a cabinet, and 1/8 globally) of local memory bandwidth. Providing a global memory address space with nearly flat memory bandwidth simplifies programming by reducing the importance of partitioning and by making it easier to load balance computations.

Our effort is not aimed at developing the computer itself, but rather it is focused on demonstrating feasibility, developing enabling hardware and software technology, and reducing the risk of a full development effort. A full development effort would be a much larger undertaking than our present project. However, by laying the technical foundation, the current effort will likely facilitate full-scale development, under separate funding.

FY03 Accomplishments for the Streaming Supercomputer group

During the first half of FY03, we focused on rebuilding our software infrastructure, demonstrating the performance of streaming on a larger scale, and resolving key architectural questions. During FY02, the first year of the project, we built a software infrastructure based on a *metacompiler*. This approach enabled us to get up to speed quickly: building a working implementation of the Brook programming language and demonstrating three small applications in the course of a single year. Unfortunately, the metacompiler cannot meet the long-term needs of the project. It cannot be used to perform kernel and stream optimization analyses required as we move forward.

After a survey and evaluation of alternative approaches, we have selected the open research compiler (ORC) as a foundation for our programming tools. During the remainder of FY03 we plan to modify this compiler to support Brook (and also Brooktran – a Fortran variant of Brook) and to implement a number of key optimizations using this compiler framework. The unanticipated need to replace our compiler infrastructure has delayed our overall progress by about two quarters. The applications and architecture portions of the project are also impacted, as they are dependent on the compiler infrastructure.

During FY02 we demonstrated the feasibility and advantages of streaming by simulating the execution of three simple 2-D applications on a single node of a streaming supercomputer. During FY03, we expect to demonstrate the feasibility and efficiency of streaming on larger scale applications and machine models. We are building several 3-D streaming applications to demonstrate that stream processing can handle applications of this scale and to identify issues related to application scaling. In a similar manner, we are simulating the execution of applications on a multi-node streaming supercomputer to demonstrate scaling beyond a single node and to expose issues related to scaling machine size. A key goal is to simulate at least one 3-D application on a multi-node streaming supercomputer by the end of FY03.

We have started a series of point studies aimed at resolving key architectural issues. For example, we have simulated a set of alternative stream register file (SRF) organizations to determine the most efficient organization. This study revealed that providing cross-lane indexing in the SRF gives significant performance advantages for codes with certain access patterns. The study also shows that indexing is inexpensive and subsumes the scratchpad that was previously a part of our strawman architecture. Other studies that we plan to complete during FY03 address program-assisted caching, processor aspect ratio, synchronization mechanisms, and scatter-add memory mechanisms. We expect these studies to lead to an architecture that is low-risk and supportable by experimental evidence.

During FY03 we have launched our search for an industrial partner by holding meetings with representatives of Cray, SGI, and Sun. We also plan to meet with IBM and HP before the end of FY03. These initial meetings are intended to inform the companies about the technology and to open the discussion of possible collaboration. The response has been lukewarm so far. However, we are guardedly optimistic that one or more potential partners will become more interested as our work progresses and the argument becomes more compelling.

FY04 Goals for the Streaming Supercomputer Group

The major goal for FY04 is identifying an industrial partner to help us proceed with the detailed design of the streaming supercomputer in FY05. Toward this end, we plan to complete: a detailed micro architecture, a working compiler, the design (but not implementation) of an operating system, and convincing application demonstrations. In this way we will show the advantage of stream processing along with solutions to potential issues with its implementation.

To complete the micro architecture, we plan to complete all of the remaining architecture studies during FY04. These studies depend on realistic applications, and an optimizing compiler. Hence, we also plan to complete a final specification for the Brook programming language and the stream virtual machine in FY04, and to extend our compiler to handle the full Brook language with basic optimizations. During FY04 we will extend our 3-D model applications and will begin work on porting the actual CITS codes (URANS and LES) to the streaming supercomputer.

We plan to develop a design for an operating system and perhaps prototype its key components. This system will most likely involve running a simple kernel that provides only process and memory management on each node of the machine; with a full operating system (most likely Linux) running on designated I/O nodes providing full operating system services. In particular, we plan to work out in detail the parallel I/O system, and the system support (checkpoint, restart, diagnostics, etc) for guaranteeing reliability and availability.

University of Chicago – Center for Astrophysical Flash Phenomena

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In addition, overall collaboration with Argonne National Laboratory (ANL) is overseen by R. Stevens, Division Director of Mathematical and Computer Sciences at ANL.

Project Description. The goal of the Center is to solve the long-standing problem of thermonuclear flashes on the surfaces of compact stars, such as neutron stars (X-ray bursts) and white dwarfs (novae), and in the interior of white dwarfs (Type Ia supernovae). Physical phenomena in this problem include: accretion flow onto the surfaces of these compact stars; shear flow and Rayleigh-Taylor instabilities on the stellar surfaces and interiors; ignition of nuclear burning under conditions leading to convection; and either deflagration or detonation, stellar envelope expansion, and the possible creation of a common envelope binary star system. The Center's scientific goal is realized by means of the construction of the multi-dimensional, multi-physics, simulation "*Flash"* Code.

Collaboration with other Universities. The Center has two subcontracts with other university groups:

- **RPI:** This collaboration has focused on exploring the use of unstructured grids and continuous Galerkin methods as an alternative hydrodynamic solver. This collaboration will terminate at the end of FY03 due to budgetary constraints.
- **Univ. of Arizona:** UofA is a "beta test site" for the *Flash* code (they use the *Flash* code for astrophysical problems that are related to, but not identical with, the Center problems). Tthey have also collaborated with us in validation studies.

Sub-Project Descriptions:

Astrophysics. The Center is addressing three key astrophysical problems: novae, Type Ia supernovae, and X-ray bursts. The primary scientific objectives of the Center during the next two years will be to carry out large-scale, integrated, multi-physics simulations of (1) novae; and (2) secondarily, Type Ia supernovae. Analytic and numerical studies of X-ray bursts will be carried out during the next two years, but large-scale, integrated, multi-physics simulations of X-ray bursts will not be a priority.

The focus of the simulations that the Astro group will carry out on novae during the next two years will be primarily to

- understand the long smoldering phase that occurs prior to thermonuclear runaway in novae; and secondarily to
- study the thermonuclear runaway phase, and the resulting explosion.

The choice of the smoldering phase as the primary focus of nova simulations during the next two years is based on the fact that very little work has been done on this phase, yet the properties of the eventual explosion depend on the starting conditions set by the smoldering phase -- which sets the initial conditions for thermonuclear runaway.

Specific milestones for the nova simulations for 2003 are (1) 3D simulations of wind-wave mixing, and (2) 1D global simulations of novae. Both have been achieved. We have extracted from extensive 2D and three 3D wind-wave mixing simulations the information that we needed in order to construct a set of three physically self-consistent sub-grid models of the mixing, and have completed a set of 1D nova calculations, using these sub-grid models, that are highly informative.

Specific milestones for the nova simulations for 2004 are: (1) 3D global simulations of novae, and (2) making more definitive statements about the effects of our sub-grid mixing model. Milestones for the out years include (1) calculating the nucleosynthetic yield of the nova outburst; and (2) radiation transfer calculations that will allow us to compare the light curve and spectrum of the nova outburst with observations.

The focus of the simulations that the Astro group will carry out on Type Ia supernovae during the next two years will be primarily to

- study the thermonuclear runaway phase; and secondarily to
- understand the smoldering phase that occurs prior to the explosion.

Specific milestones for the Type Ia supernova simulations for 2003 are: (1) 2D and 3D simulations of the turbulent deflagration phase; (2) demonstrating convergence of the explosion energy with resolution, and that the explosion energy is as large as is observed; and (3) stating why or why not 2D simulations suffice.

Early in FY03, we made considerable progress toward these milestones. We have achieved a stable 1D white dwarf starting model, and much more stable 2D and 3D white dwarf starting models than previously available. We are undertaking 2D and 3D detonation simulations using

these models as a warm-up exercise for the 2D and 3D deflagration calculations to be initiatee in June of 2003, using the reaction-diffusion front tracking algorithm that is being developed by the Comp Phys group (see below).

Specific milestones for the Type Ia supernova simulations for 2004 are: (1) 3D simulations of the smoldering convective phase from about 30 minutes before runaway to runaway, and (2) making a statement about where ignition occurs, and how many ignition points there are. Milestones for the out years include: (1) 2D and 3D simulations of the smoldering convective phase from several days before runaway to runaway;
(2) detonating the white dwarf at various times during the turbulent deflagration phase, in order to pin down when and where the detonation must occur, if the explosion energy and the abundances of intermediate and iron group nuclei are to match those that are observed; and (3) radiation transfer calculations that will allow us to compare in some detail the light curve and spectrum of the nova outburst with observations.

Computational Physics and Validation. The highest priority Comp Physics and Validation milestones for 2003 are to choose, develop, write, and implement

- an interface tracking scheme; and
- a compressible, low-Mach number, implicit hydro solver.

These priorities derive from the computational physics capabilities needed in the *Flash* code in order to fulfill the astrophysics plan. These milestones are well on the way to being achieved. A decision has been made to use a reaction-diffusion front tracking algorithm. A 1D algorithm has been written, and is being tested. The results are very promising. Generalizing the algorithm to 2D and 3D will be straightforward, once it has been fully tested in 1D. A decision has been made to use a BIC implicit hydro solver. A prototype 1D BIC implicit hydro solver has been written and fully tested. A 2D version has been written and is currently being tested. The remaining tasks are to test the 3D solver (May - June 2003), and to begin astrophysical tests of the 3D solver (July 2003).

Specific milestones for the Comp Physics and Validation group for 2004 are

- computational modules: (1) to complete implementation of the low Mach number implicit solver; and to choose, develop, write, and implement (2) an additional front tracking module (most likely based on the level set or volume-of-fluid methods), (3) a multi-fluid MHD module, and (4) a projection-based low-Mach flow solver;
- applications: to develop a data interface for the radiation transfer code that will be used to calculate spectra/light curves from our Type Ia SN models; and
- validation: (1) to publish the results of our collaboration with Bob Benjamin at LANL on the shock-cylinder experiments, and (2) extend our validation work to laser-driven experiments at LLNL, most likely with Bruce Remington.

Comp Phys and Validation milestones for the out years include: (1) a fully relativistic MHD solver; (2) a multi-physics implicit solver; (3) subgrid models for flames (along the lines of the Active Turbulent Combustion model developed by Alan Kerstin); and (4) continuing our validation studies.

Code. The highest priority Code group milestones for 2003 are to

- develop a fast, adaptive mesh refinement elliptic solver; and
- migrate physics modules to a second (new) branch of the *Flash* code, so that they can be used with the compressible, low-Mach number, implicit hydro solver.

These milestones have largely been achieved. *Flash* 2.3 is scheduled for release on 1 June 2003. New capabilities in it will include: (1) optimized multi-grid for a uniform grid, (2) optimizations to an adaptive mesh refinement multi-grid, (3) support for parallel NetCDF I/O format, (4) FT-based Poisson solvers with arbitrary boundaries, (5) FFT-based solvers on adaptive mesh refinement grid, and (6) support for implicit solvers.
Specification of *Flash* 3.0 is scheduled for 15 May 2003.

Code milestones for 2004 include:

- achievement of *Flash* 3.0 development goals, which include: (1) reorganized database APO, (2) increased module inter-dependency using mappers, (3) completely restructured/generalized drivers to more easily support implicit methods, (4) packaged portable 3D visualization tool, (5) support for FFT-based solvers (Poisson, etc.), (6) support for auto-generated xml-based performance summary, (7) Paramesh 3.0, (8) full support for spherical and cylindrical geometries, (9) more complete built-in memory diagnostics, (10) developer's guide, and (11) module unit testing.
- successful interactions with (1) the Comp Phys group to ensure framework support for new algorithms (in particular, the front tracking and implicit hydro modules), (2) the CS group to exploit Jumpshot and Autopack for multigrid optimizations, and (3) the Astro group to support, document, maintain, and bug-track source code.

Computer Science. The highest priority CS milestone for 2003 is to construct a visualization "pipeline" for the large-scale, integrated, multi-physics simulations that the Astro group will be carrying out during the next two years.

Significant progress has been made toward this milestone. The CS group has deployed the initial version of our FLASH desktop tool and has begun receiving feedback from *Flash* code users. The CS group also began development of a collaborative visualization tool that exploits the Access Grid collaboration environment. In FY '04 the CS group will complete development of these tools.

Other significant CS group milestones achieved in 2003 include:

- scalable performance and I/O: (1) completed the SLOG2 scalable log file format and libraries and (2) released Jumpshot-4, and (3) began to implement a parallel version of NetCDF, which provides opportunities for greater performance than HDF5;
- numerical libraries: began incorporating *Autopack* into provisional versions of the *Flash* code in order to experiment with performance;
- distributed computing: established a Web-based tool at the FLASH Center for discovery of the availability of computing resources, and deployed GridFTP as a tool for moving files to the Center from the ASCI sites.

CS milestones for 2004 include: (1) extending both SLOG2 and Jumpshot to deal with the functions of MPI-2, (2) completing the parallel NetCDF implementation and its interface into the *Flash* code as one of its I/O options, (3) incorporating *Autopack* into the *Flash* code, and (4) completing a remote job-submission tool that will make it easier for Flash Center researchers to use remote facilities.

Basic Physics: Basic Physics group accomplishments in 2003 include: (1) establishing sufficient conditions for linear instability of fronts, including flame fronts, (2) demonstrating that fronts have bounded speed when they are confined to cylinders (although the bounds diverge as the cross-section of the cylinder increases). Goals for 2004 include: (1) extending the studies of fronts to nonlinear instabilities and connecting this work to the Astro group simulations and studying (2) fronts in compressible flows, (3) "fast" reconnection in 3D MHD, and (4) cases in which usual methods for gas dynamics (PPM included) induce pressure pulses as contact discontinuities move.

University of Illinois at Urbana/Champaign – Center for Simulation of Advanced Rockets

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Project Overview: The goal of the Center for Simulation of Advanced Rockets (CSAR) is the detailed, whole-system simulation of solid propellant rockets from first principles under both normal and abnormal operating conditions. Inherent in this simulation are requirements to accurately treat very high energy densities, extremely diverse length and time scales, complex interfaces, and reactive, turbulent, and multiphase flows.

CSAR is focusing on the reusable solid rocket motor (RSRM) of the NASA Space Transportation System, better known as the Space Shuttle, as its simulation vehicle. The RSRM is a well established commercial rocket, is globally recognized, and most importantly, design data and propellant configurations are available. The Center has a Space Act Agreement with NASA in place to share data and simulation results. Several smaller scale rockets are also simulated to provide validation data for CSAR codes. Simulations that include full geometric and materials complexity require a sequence of incremental developments—in engineering science, computer science, and systems integration—over an extended period.

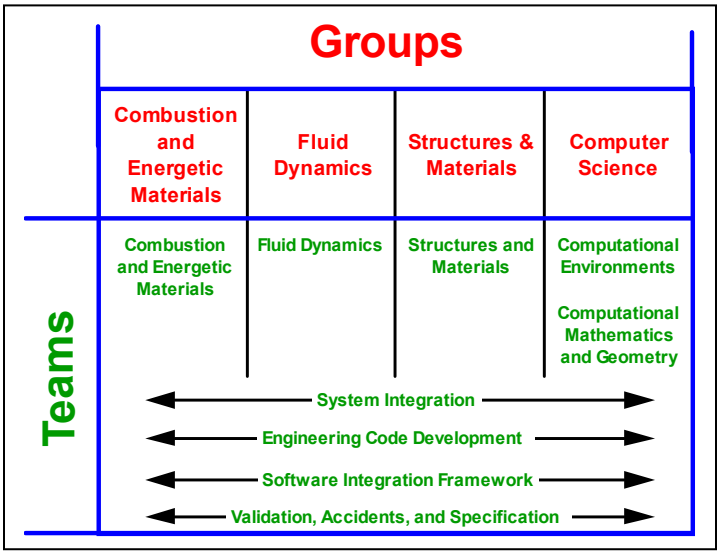
Our approach to system integration has been to develop a single executable code containing modules for the various components and an interface code for tying them together. We are following an object-oriented design methodology that hides the data structures and other internal details of the individual component codes. This simplifies development and maintenance of the interface code and the component codes, and also makes it easier to swap different versions of the same component—a critical capability for determining the most efficient algorithms and implementations.

Broadly known as *Roc** ("rock-star"), the CSAR simulation code is a fully coupled, multiphysics suite of integrated modules for 3-D simulation of solid propellant rocket performance on massively parallel computers. The suite is designed to be sufficiently general to solve any fluid/structure interaction problem. Components include fluid dynamics (*Rocflo-MP, Rocflu*), entrained particle tracking and interaction (*Rocpart, Rocsmoke*), solid mechanics (*Rocsolid, Rocfrac*), fracture (*Rocfrac*), combustion (*Rocburn, Rocfire*), and software interface codes for

coupling and mesh association (*Roccom, Rocman, Rocface*). An initial implementation of *Roc** (GEN1), which was operational at the end of 2000, provided a simplified characterization of various burn scenarios. The GEN1 code employed macroscopic models for the separate components to enable a strong focus on the definition and resolution of system integration issues. Refined, multiscale component models and advanced system integration concepts, based on lessons learned from GEN1, constitute the key features in the second-generation (GEN2) code, developed during FY01 and FY02. Continued refinement of models reflect the synthesis of fundamental, subscale studies that are critical for detailed simulations of accident scenarios and for reliable simulation of multiscale phenomena such as combustion and turbulence.

More than 100 UIUC faculty, students, and researchers currently contribute to the success of the Center. An External Advisory Board (EAB) provides critical guidance in rocket simulation and computational science. EAB membership is drawn from the DOE NNSA/DP laboratories, Department of Defense research agencies, NASA, and academia, as well as the commercial rocket industry, and the computer hardware and software industries. The DOE-supplied budget has been sufficient to maintain an aggressive research program. In addition, the University of Illinois has provided funds for ancillary research expenditures, computer workstations, and facility renovation.

Center Management and Staffing Plan: The whole-system simulation of solid propellant rockets requires the close interaction of the four CSAR Research Groups: Combustion and Energetic Materials, Fluid Dynamics, Structures and Materials, and Computer Science. Nine Research Teams have been identified to address the specific needs of each aspect of the simulation. Five of the research teams operate within the loose bounds of the group structure; four research teams function as crosscutting programs.



Major Integrated Rocket Simulations and Validation Studies

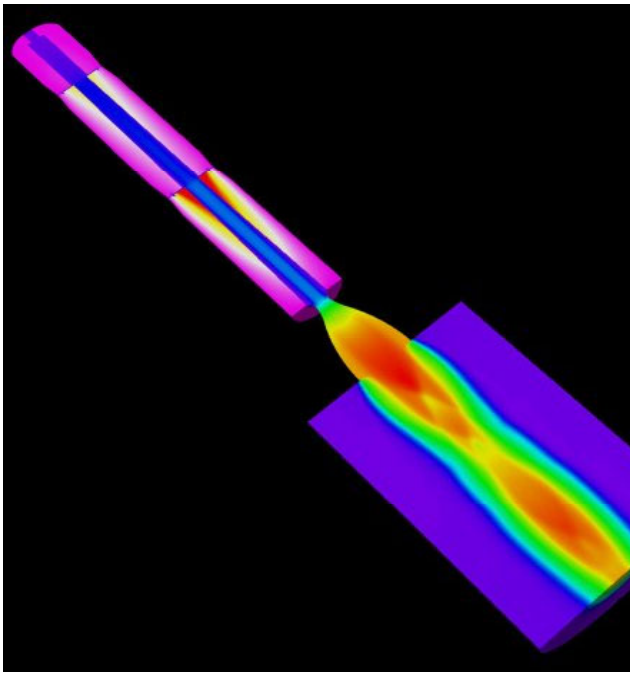
RSRM simulations — Semi-annual simulations of RSRM are planned to exercise the then-most recent features of the simulation. These simulations will increase in complexity and machine demand through the end of DOE/NNSA DP support, concluding with a 10,000 +/- processor simulation run. — March 2004, September 2004

Attitude Control Motors — Atlantic Research Corporation (ARC) has recently supplied us with detailed design and experimental data for small guidance rockets as a validation test for our code. Simulating these small motors will require accurately modeling ignition transients and adapting meshes automatically as the propellant burns away completely. There are flexible baffles in some of these motors that divide and reunite the fluid domain as the system evolves. An advanced 3-D remeshing capability will be required for such topology changes. — December 2003

Gravitational/inertia effects (for lab scale rockets) — This topic is of particular interest to the rocket industry and will exercise the full 3-D nature of the code. *Roc** will be extended to include gravitational/inertial terms enabling simulations of full 3-D flight dynamics. — June 2004

RSRM *Challenger* accident (simulate flow past O-rings) — This problem requires the structures solver to handle contact. Fluids domain topology changes when the gas begins to pass around the O-ring. — Late 2004

Titan IV case rupture accident — In this simulation, the pressure builds up until the case fails. In test firing an early design, a rocket motor exploded violently destroying the test stand, but there was no propellant detonation. (By the time we implement the required remeshing capability, we expect to have an advanced material model for the propellant that includes the effects of voids and dewetting.) — 2005



Results from fully coupled, 3-D simulation of Titan IV solid rocket booster 0.36 seconds after ignition. Gas flowing around joint slots causes propellant to be pulled inward, locally restricting gas flow. In test firing of this early design, propellant deformed more than expected, causing pressure to build up and destroy rocket 1.58 seconds after ignition.

RSRM complete normal burn — The ignition transients for the Space Shuttle booster are well characterized in the open literature, and we have access to extensive test data. An especially difficult aspect of simulating the entire history of a large motor is reducing the run time. For a fluids mesh that is fine enough to allow accurate turbulence modeling, for example, *time zooming* techniques under consideration will be required to reach 120 seconds of physical problem time. — 2006

Accomplishments in the Center during FY03 include:

- extended verification and validation of integrated code using NASA RSRM, Titan IV, and commercial guidance rocket datasets
- studied and resolved element instabilities resulting from high applied loads (pressures above the elastic modulus) on near-incompressible materials
- developed new ignition model based on heat flux and radiant properties
- developed initial code for combustion simulation of aluminized propellants using level set methods
- examined combustion instabilities in propellant cracks
- integrated new unstructured simulation code and reformulated structured simulation code for rocket bore fluid dynamics
- implemented new turbulence module in fluid dynamics simulation code

- integrated adaptive MPI and virtual processor methods in parallel programming environment
- improved significantly both scalability and single-node performance of integrated simulation code through detailed performance monitoring and analysis.

Key project goals for FY04 include:

- incorporate LES turbulence model in *Rocflo-MP*
- capture 3-D vortex shedding in RSRM simulations downstream of inter-segment inhibitors
- fully integrate unstructured mesh fluids solver — *Rocflu* —in *Roc**
- add gravitational body forces to the *Rocflo-MP* and *Rocfrac* modules
- resolve propellant "walkback" in structures modules
- verify automatic insertion of cohesive elements in *Rocfrac*
- complete parallel implementation of remeshing for tetrahedral meshes.

University of Utah – Center for the Simulation of Accidental Fires and Explosions (C-SAFE)

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Project Overview: The objective of C-SAFE is to provide a scalable, high-performance computational simulation system composed of a problem solving environment in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, optimization, computational steering, visualization, and experimental data validation. During FY03 significant effort was directed toward reconfiguring our software integration strategy to support the full, end-to-end simulation of an explosion of a steel container of PBX9501 immersed in a hydrocarbon pool fire. This effort will continue into FY04, along with many other supporting tasks and milestones, as detailed below.

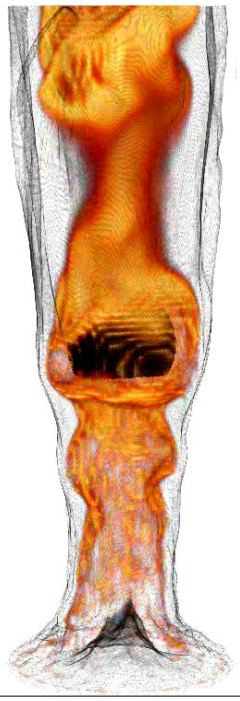

Fig. 1 - Volume rendered temperature field of a 1 m heptane pool fire with a 30 cm dia. steel cylinder containing primary explosive HMX.

Project Descriptions

Our Uintah simulation software is designed to support team integration by separating parallelism from the application component scientific codes. The major ongoing projects within the Computer Science team to support this integration strategy are:

- Problem Solving Environment (PSE) - provide a common software infrastructure, environment and version control for large-scale simulation code development including basic data structures, meshing components, parallelization, scaling and performance analysis tools.
- Visualization - develop techniques for interactive large-scale data visualization and analysis for both simulation data (especially Fire Spread and Container Dynamics) and performance analysis.

- Adaptive Mesh Refinement (AMR) - help achieve overall simulation goals with sufficiently accurate techniques and with appropriate refinement criteria and scalable load balancing.

The focus of the Fire Spread (FS) team is to use large eddy simulations (LES) to simulate the temporal heat flux and emissions in and around an evolving hydrocarbon pool fire in the presence of solid structures. Figure 1 illustrates the current state of the simulation capability. The fire framework components currently planned for FY04 by the FS team include:

- Algorithmic development for long-time scale (>3 minutes) fire simulations
- Simulation tools for radiative heat transfer with participating media (including scattering)
- Model development for the physics and chemistry at the subgrid scale in the fire and at the boundaries of the fire and the solid structures
- Local mesh refinement methods for improving accuracy of the LES fire and structure
- Methods to perform validation and error budget analyses for the fire simulation in the presence of structures.

The Container Dynamics group focuses on developing algorithms for tightly coupled fluid-structure interaction (FSI) capabilities required to simulate the wide range of physical phenomena that occur through heating confined energetic materials. The capabilities must handle thermal and fluid transport, chemical decomposition (solid $\rightarrow$ gas), rigorous description of solid mechanics and compressible gas dynamics, strong coupling between the solid and fluid fields including feedback to the fire, and the ability to handle a wide range in temporal scales (minutes to milliseconds). Current efforts address the following areas:

- MPM algorithm development - An implicit version of MPM has been implemented and tested. Work in progress includes improving efficiency and scalability, as well as implementing the necessary tangent modulus for a wider range of material models.
- Semi-implicit CFD development - A single material semi-implicit version (with respect to pressure). Current work is focused on the multi-material version.
- Constitutive modeling of metal - Our target scenario involves subjecting metals to extreme strain rates at elevated temperatures. Current efforts in this area involve developing a general framework that can handle a wide range response to thermal and mechanical loading. Capabilities must include accurate description of large deformations, rotations, and strains for a wide range of strain rates, and damage.
- Fracture in MPM - Algorithms for describing cracks (with contact), evaluating key fracture parameters, and propagating cracks are being developed and incorporated into MPM. Efforts are underway to incorporate realistic material models into the MPM fracture methods to model crack propagation in both elastic and inelastic materials.

The Molecular Fundamentals team provides the scientific underpinnings for subgrid-scale models that allow the simulation to capture accurate underlying chemical and physical properties of the materials in the computational domain. Some of the specific ongoing tasks are:

- Kinetics of Soot Formation
- Optical Properties of Soot
- Reaction Rate Constant Calculations from Quantum Molecular Dynamics
- Combustion of Hydrocarbon Fuels
- Reaction Mechanism Reduction

- Reaction Mechanisms for Condensed-phase HMX Decomposition
- Further Development of Quantum Molecular Dynamics for Energetic Materials
- Combustion Simulations with Advanced Kinetics
- Viscoelastic Properties of PBX-9501 Binder
- Coarse-grained Simulations of Model Estane/HMX/Plasticizer Systems
- Mesoscale Simulations of Granular Materials
- Development of New Composite Properties Homogenization
- Development of Methods for the Efficient Calculation of Material Properties

Validation has been a major theme since the inception of the Center. Current tasks include:

- Soot Formation/Characterization from Liquid Fuels - Soot samples will be created from model compounds, JP-8, and JP-8 surrogates for subsequent characterization of molecular structures using solid-state NMR analysis.
- Vapor Liquid Interface Studies - Parameters that can affect the vapor composition will be studied in the pool fire test facility. Model validation data will be obtained including spatially resolved data on soot concentration and particle size distribution in the pool fire.
- Container-HE Material Interface Studies - Tests carried out in conjunction with Thiokol Propulsion will focus on the influence of surface heat flux and other parameters on time-to-explosion and violence of the explosion.
- Soot Surface Growth and Oxidation - Surface growth and oxidation of soot will be studied in a two-stage experiment that uncouples the soot formation and oxidation steps.
- Characterization of Laminar Diffusion Flames - A Wolfhard-Parker burner will be used to test soot formation and transport, as well as absorption and emission coefficients.
- Fire Container Interface - The impact of the deposition of soot on the container surface will be investigated to determine changes in surface emissivity and the creation of a conductive barrier.
- Soot Agglomeration/Oxidation Model – Development of a mathematical model for the description of soot particle agglomeration, growth by condensation, fragmentation and oxidation for neutral or charged soot particles.

Accomplishments in FY03

- Completed a baseline integrated Fire/MPM code in the Uintah Computational Framework
- Performed large-scale 3D visualizations (Fire Spread and Container Dynamics)
- The Uintah PSE was ported successfully to the LLNL IBM SP platform
- The initial phase of the LANL Compaq Q machine port was completed
- The basic mesh refinement and AMR strategies were defined by the Computer Science, Fire Spread and Container Dynamics teams
- Created the basic AMR UCF components
- Performance study of Uintah codes
- Completed a coupled simulation with a heptane pool fire and a steel container of HMX through to explosion with quantitative validation for time to explosion compared to CSAFE experiments
- Demonstrated a large pool fire (18.5 m diameter) simulation with a crosswind (5 m/s)

- Demonstrated and validated an algorithm to compute heat flux to a container for long-time scale fire simulations by performing a calculation at multiple resolutions for a fire that ran for in excess of 2 minutes of fire time
- Demonstrated methods for incorporating realistic chemistry in the simulation of fire and explosions by the use of subgrid models based on a heptane and soot chemical kinetic mechanism involving 1538 chemical reactions, and an HMX chemical kinetic mechanism with 237 reactions. Also performed validation studies to begin error quantification on both mechanisms
- Constitutive model development; Incorporation of general hypo- and hyper-elastic-plastic constitutive models, providing the framework for strain, strain-rate and temperature dependence. Implementations include Johnson-Cook plasticity with damage and Mechanical-Threshold Stress plasticity. Damage implemented and tested with a range of "particle erosion" methods.
- Implicit MPM was incorporated into the UCF
- Multi-material CFD. Implementation of semi-implicit method for single materials. Significant algorithm developments and improvements for MPM-ICE coupling of large deformation FSI problems and modeling energy exchange between materials
- Cracks and crack propagation in MPM. A new crack description algorithm was implemented, yielding better overall computational efficiency, accuracy in computing crack growth parameters, and more rigorous treatment of crack contact
- Demonstration of full end-to-end simulation capabilities. A simulation of a container in a heated jet was conducted to demonstrate the required pieces of our end-to-end simulation can be run in a single framework
- Large-scale simulations of heated containers undergoing large pressure induced deformations
- Perfected and applied a Molecular Dynamics (MD) and Kinetic Monte Carlo (KMC) approach for soot formation in flames, yielding a molecular perspective on these processes for the first time
- Implemented Time-Dependent Density Functional Theory (TDDFT) to calculate the optical properties of precursor molecules to soot
- Obtained and began implementation of the MIT RIOT code for mechanism reduction for hydrocarbon fuel combustion
- Calculated the condensed-phase free energy barriers for NO2 dissociation and HONO elimination in HMX using first-principles quantum MD, yielding important insight into the possible initiation step(s) for this material
- Calculated important material properties for HMX, Estane, and binder using MD methods outside of the accessible range of experiments
- Working soot agglomeration model and first-generation oxidation model including the effect of particle charge
- Quantification of the impact of surface heat flux and internal solid voidage on explosion violence for PBX9501
- Data were obtained on molecular structures of intermediate soot and precursor species, and these data provided insights on the transformation mechanisms for alkane and aromatic species into soot precursors

- More clearly delineated the effect of local oxygen and temperature on formation of soot in JP-8 diffusion flames
- Developed experimental capability for measuring soot deposition on a container engulfed in pool fires

Planned Work in FY04

- Continued incorporation of Fire Spread and Container Dynamics modules and Molecular Fundamentals results into the integrated multi-physics code (i.e., an end-to-end application and better exploration of efficient spatial-temporal coupling of fluids, chemistry, radiation and container dynamics)
- Continue development of large-scale data management and migration tools
- Continue development of scalable load-balancing strategies, especially with respect to particle-based simulations, AMR and cluster machines
- Continue improvement of visualization tool stability and scalability (specifically for face-based data, MPM surface vis, and parallel and remote vis)
- Continued design, maintenance and upgrade of the Uintah software and the Uintah Computational Framework for the entire C-SAFE project.
- Develop implicit time solvers for the fire simulation to provide improved accuracy and reliability (robustness) over explicit methods by reducing operator splitting error.
- Develop higher order time differencing methods for fire to provide better accuracy and reliability for time marching methods. The higher order methods will also provide numerical error estimators for quantifying error budgets on the simulation.
- Extend the SGS reaction model to link complex chemical kinetics with SGS transport (both gas phase and soot) into the LES fire computation. The gas phase chemistry and chemical time scales are incorporated into the fire simulation through the subgrid scale reactions models. The soot is tracked in the resolved scale calculation. A heptane pool fire will be simulated. Both gas phase species as well as soot volume fraction will be compared to experimental data.
- A spectral discrete ordinates code is being developed for improving heat transfer predictions. The code will be validated against benchmarks. Coarse mesh pool fire simulations will be performed and predictions compared with experimental values to better optimize accuracy and computational time.
- Efficiency and design improvements will be made in the computer science of the SGS mixing/reaction models. This change will allow many different mixing and reaction models to be used by the LES without significantly increasing computational costs.
- The class of synthetic field subgrid closure is being explored as an improvement over conventional turbulent diffusivity methods. The 1-D turbulence model of Kerstein is of primary consideration at this time.
- Quantitative evaluation/validation of LES mixing & reaction models using DNS.
- Developing mesh refinement algorithm for fire and to show a proof of concept by applying it to a simple pool fire simulation.
- Develop a method for embedding complex geometry on the fixed, Eulerian mesh and modeling the fluid/structure interaction. The method will be validated by comparison to pedagogical geometries then extended to modeling complex geometries in fires.
- Further develop and validate the SGS model for ignition and transient combustion of HMX.

- Perform parametric simulations involving a fire and container HMX to study the effect of location in the fire on time to explosion.
- Validating fire simulation results by comparing with experimental data.
- Algorithm development in support of end-to-end simulation scenario. The multi-material ICE-MPM algorithm has been developed within CD. A major focus of planned work in FY04 in CD is directed to algorithm and model development for the fire-container coupling. Aspects of this work involve completion of the semi implicit ICE algorithm, coupling of ICE to implicit MPM, boundary conditions, and collaboration among CD, CS and FS on incorporating ARCHES fire modules into the ICE-MPM framework.
- Constitutive model development. Efforts will be focused on metals at high strain, strain-rates, and temperatures.
- Fracture. Development and incorporation of 3-D propagation in the UCF. Development of appropriate fracture criteria for inelastic materials.
- Develop and begin to implement a new unified MD strategy for soot growth, complete with accurate rate constants. Combine these calculations with TDDFT calculations to characterize the optical properties of the emerging soot particles. Pass on these calculated molecular properties to the Fire Spread soot modeling team.
- Develop and implement a novel MD/MPM interface for integrating MD properties for PBX9501 into the MPM Container Dynamics code. This methodology will employ a multi-scale homogenization procedure.
- Detailed soot deposition measurements to quantify impact on heat flux to container in a sooting pool fire, for use in subsequent model development.
- Detailed species characterization for solids and liquid extracts from soot formed during the combustion of JP-8, surrogate JP-8 and model compounds, to facilitate kinetic mechanism development.